

Fracture in III-Nitride Alloys Permits Dislocations to Relieve Tensile Stress

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Motivation—Aluminum gallium nitride (AlGaN) is an alloy of GaN and AlN that offers significant potential for use in ultraviolet (UV) light emitting devices. Such devices are needed in a variety of critical sensing applications. AlGaN is typically grown epitaxially upon GaN epilayers in a state of tensile stress due to the difference in lattice parameters. This can lead to fracture of the AlGaN, which is deleterious to device operation. Unfortunately, a great deal of confusion permeates the III-nitride literature with regard to the energetics and kinetics of fracture processes.

Accomplishment—We performed real-time stress measurements during chemical vapor deposition of epitaxial AlGaN layers on GaN in a rotating disk reactor. These novel experiments required synchronization of our Multi-beam Optical Stress Sensor (MOSS), a wafer-curvature monitor developed at Sandia, with a sample spinning 1200 times per minute. Our results clearly demonstrated that relaxation occurred during growth (rather than after), identified the critical thickness for onset of fracture, and determined the overall degree of strain relaxation. The latter revealed the surprising result that the observed crack densities accounted for a small fraction of the relaxation, directly implying the presence of a different stress-relieving defect (Fig. 1). Subsequent transmission electron microscopy exposed the presence of a dense array of misfit dislocations at the AlGaN/GaN interface that accounted for the majority of the stress relaxation. The cracks do play an important role, however, in that they permit facile propagation of misfit dislocations

in a materials system for which such processes are otherwise highly constrained. The MOSS measurements also mapped out the critical thickness for fracture as a function of the alloy composition. We demonstrated that this data could be consistently described by a simple fracture energetics model (Fig. 2). In some films we observed metastable growth, i.e., the formation of films that are thermodynamically able to crack but are kinetically constrained from doing so. Finally, we showed that cracks can be dynamically overgrown and buried during film deposition. This process may be responsible for erroneous conclusions in previous literature reports that fracture occurs during cooldown after growth, which was inferred from cracks that appeared to propagate upward from the AlGaN/GaN interface.

Significance—Our work immediately raises the question of whether it is really cracks that cause problems for devices, or whether it is, in fact, the dense misfit dislocation array, whose presence has not been recognized previously. This issue clearly has consequences for how devices are designed. Furthermore, our measurements of the critical thickness boundary and metastability regions will help guide the design of process flows in order to obtain low defect density structures. The ability to overgrow cracks might lead to new growth schemes to reduce crack densities within the active layers of devices. Last, but not least, we have demonstrated that curvature-based stress measurement serves as a valuable diagnostic for real-time process control and characterization during chemical vapor deposition.

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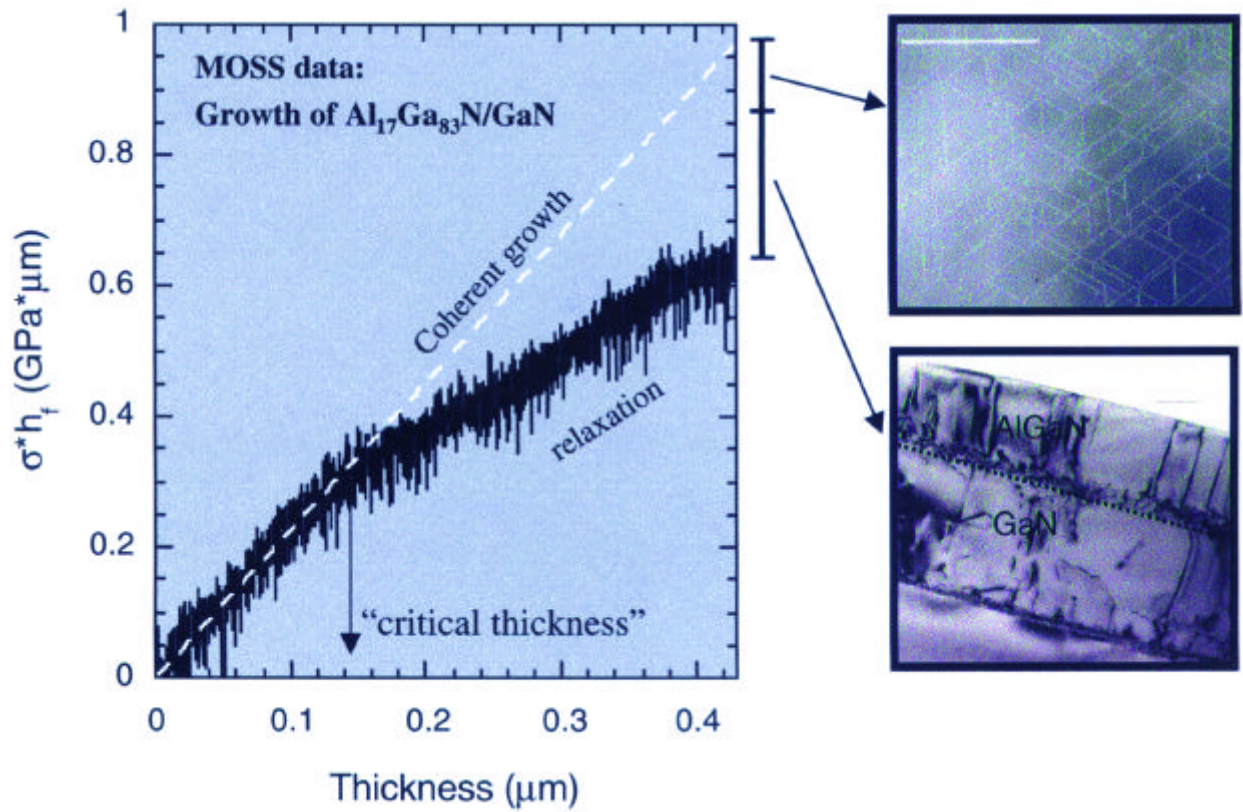


Figure 1. Real-time data on stress evolution during AlGaIn growth on GaN. The bars represent the amount of stress relaxed by cracks (upper right) and misfit dislocations (lower right).

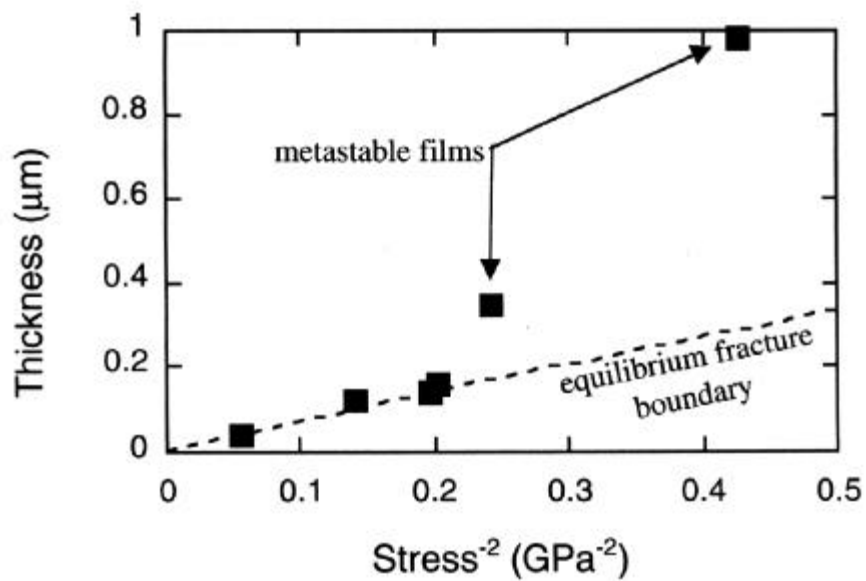


Figure 2. The measured critical thickness for fracture in $\text{Al}_{1-x}\text{Ga}_x\text{N}$ alloys. The dashed line is the calculated equilibrium critical thickness using a simple energetic theory of fracture.